Crystal structure of 4,5,2',3'-tetrahydro-4-(1,1-dimethylethyl)-1,1',3'-trimethylspiro-{[1*H*][1,2,3]-triazole-5,2'-[1*H*]-benzimidazole}, [C₆H₄N₂(CH₃)₂]C[CHN₃(CH₃)(C₄H₉)]

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Table 1. Data collection and handling.

Crystal:	colourless prism, size 0.25 × 0.75 × 0.2 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.70 cm ⁻¹
Diffractometer, scan mode:	Nicolet R3m/V, Wyckoff
2 $\theta_{\max}$:	55°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	2075, 2052
Criterion for F_{obs} , $N(hkl)_{\text{gt}}$:	$F_{\text{obs}} > 3 \sigma(F_{\text{obs}})$, 1450
$N(\text{param})_{\text{refined}}$:	181
Program:	SHELXTL-plus [3]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
H(1A)	4a	-0.2858(5)	0.6981(3)	0.1668(7)	0.08
H(1B)	4a	-0.2147(5)	0.6928(3)	0.3417(7)	0.08
H(1C)	4a	-0.2892(5)	0.6273(3)	0.2692(7)	0.08
H(4A)	4a	0.0874(5)	0.6479(3)	-0.0481(6)	0.08
H(6A)	4a	-0.1835(5)	0.5068(2)	0.0434(6)	0.08
H(6B)	4a	-0.2900(5)	0.4956(2)	-0.0959(6)	0.08
H(6C)	4a	-0.3211(5)	0.5413(2)	0.0645(6)	0.08
H(8A)	4a	-0.4493(5)	0.5696(2)	-0.2595(6)	0.08
H(9A)	4a	-0.5572(5)	0.6583(3)	-0.4166(6)	0.08
H(10A)	4a	-0.4681(5)	0.7700(3)	-0.4430(6)	0.08
H(11A)	4a	-0.2648(5)	0.7979(2)	-0.3132(6)	0.08
H(13A)	4a	0.0189(6)	0.7534(2)	-0.0163(7)	0.08
H(13B)	4a	-0.1142(6)	0.7936(2)	-0.0089(7)	0.08
H(13C)	4a	-0.0363(6)	0.7900(2)	-0.1790(7)	0.08
H(41A)	4a	0.0978(7)	0.6465(3)	-0.3396(6)	0.08
H(41B)	4a	-0.0238(7)	0.5975(3)	-0.3625(6)	0.08
H(41C)	4a	0.1131(7)	0.5725(3)	-0.4260(6)	0.08
H(42A)	4a	-0.0443(6)	0.4886(2)	-0.1915(7)	0.08
H(42B)	4a	0.0657(6)	0.4684(2)	-0.0631(7)	0.08
H(42C)	4a	0.0919(6)	0.4638(2)	-0.2580(7)	0.08
H(43A)	4a	0.2747(5)	0.6095(3)	-0.1350(8)	0.08
H(43B)	4a	0.2820(5)	0.5357(3)	-0.2240(8)	0.08
H(43C)	4a	0.2559(5)	0.5403(3)	-0.0291(8)	0.08

Abstract

C₁₅H₂₃N₅, orthorhombic, $P2_12_12_1$ (No. 19), $a = 10.282(4)$ Å, $b = 18.946(5)$ Å, $c = 7.910(3)$ Å, $V = 1540.8$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.067$, $wR(F) = 0.057$, $T = 293$ K.

Source of material

The title compound was prepared in 87% yield, according to [1], from methyl azide and 1,3-dimethyl-2-(2,2-dimethylpropylidene)-2,3-dihydro-1*H*-benzimidazole [2], in benzene solution (14 h, 275 K). Recrystallization of the product from diethyl ether/pentane (1:2) afforded colourless prisms, mp 396 K – 398 K.

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(1)	4a	-0.1205(4)	0.6445(2)	0.1557(5)	0.062(3)	0.080(3)	0.058(3)	0.014(2)	-0.002(2)	-0.012(2)
C(1)	4a	-0.2373(5)	0.6677(3)	0.2405(7)	0.077(4)	0.085(4)	0.080(4)	0.007(3)	0.014(4)	-0.008(3)
N(2)	4a	-0.0391(5)	0.6013(2)	0.2388(5)	0.077(3)	0.075(3)	0.050(2)	0.009(3)	-0.010(3)	0.002(2)
N(3)	4a	0.0487(5)	0.5771(2)	0.1423(5)	0.070(3)	0.081(3)	0.047(2)	0.017(2)	-0.008(2)	0.002(2)

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Table 3. Continued.

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(4)	4a	0.0335(5)	0.6077(3)	-0.0245(6)	0.059(3)	0.069(3)	0.062(3)	-0.003(3)	-0.005(3)	0.001(3)
C(5)	4a	-0.1075(5)	0.6357(2)	-0.0289(6)	0.061(3)	0.053(3)	0.057(3)	0.003(3)	-0.002(3)	-0.004(2)
N(6)	4a	-0.2094(4)	0.5910(2)	-0.1027(5)	0.059(3)	0.045(2)	0.064(2)	0.002(2)	-0.009(2)	0.006(2)
C(6)	4a	-0.2548(5)	0.5284(2)	-0.0153(6)	0.075(4)	0.071(3)	0.074(3)	0.001(3)	0.000(3)	0.012(3)
C(7)	4a	-0.2951(4)	0.6325(2)	-0.1983(6)	0.055(3)	0.051(3)	0.043(2)	0.008(2)	-0.000(3)	-0.001(2)
C(8)	4a	-0.4122(5)	0.6158(2)	-0.2713(6)	0.058(3)	0.061(3)	0.061(3)	0.005(3)	-0.004(3)	-0.009(2)
C(9)	4a	-0.4755(5)	0.6686(3)	-0.3634(6)	0.061(3)	0.077(3)	0.064(3)	0.014(3)	-0.007(3)	-0.008(3)
C(10)	4a	-0.4225(5)	0.7348(3)	-0.3789(6)	0.076(4)	0.069(3)	0.061(3)	0.027(3)	-0.001(3)	0.007(3)
C(11)	4a	-0.3022(5)	0.7517(2)	-0.3020(6)	0.071(4)	0.052(3)	0.063(3)	0.005(3)	0.006(3)	0.006(3)
C(12)	4a	-0.2414(5)	0.6995(2)	-0.2114(6)	0.052(3)	0.052(3)	0.055(3)	0.002(3)	0.005(3)	-0.005(2)
N(13)	4a	-0.1265(4)	0.7003(2)	-0.1224(6)	0.061(3)	0.054(2)	0.080(3)	-0.005(2)	-0.018(3)	0.004(2)
C(13)	4a	-0.0588(6)	0.7647(2)	-0.0779(7)	0.087(4)	0.063(3)	0.109(5)	-0.010(3)	-0.010(4)	-0.001(3)
C(40)	4a	0.0945(5)	0.5655(2)	-0.1702(6)	0.056(3)	0.058(3)	0.057(3)	0.004(3)	0.001(3)	0.003(2)
C(41)	4a	0.0680(7)	0.5985(3)	-0.3399(6)	0.124(6)	0.115(5)	0.061(4)	0.035(5)	0.013(4)	0.002(3)
C(42)	4a	0.0477(6)	0.4896(2)	-0.1708(7)	0.113(5)	0.079(4)	0.090(4)	-0.004(4)	0.014(5)	-0.017(3)
C(43)	4a	0.2402(5)	0.5624(3)	-0.1364(8)	0.074(4)	0.116(5)	0.102(5)	0.003(4)	0.007(4)	-0.015(4)

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